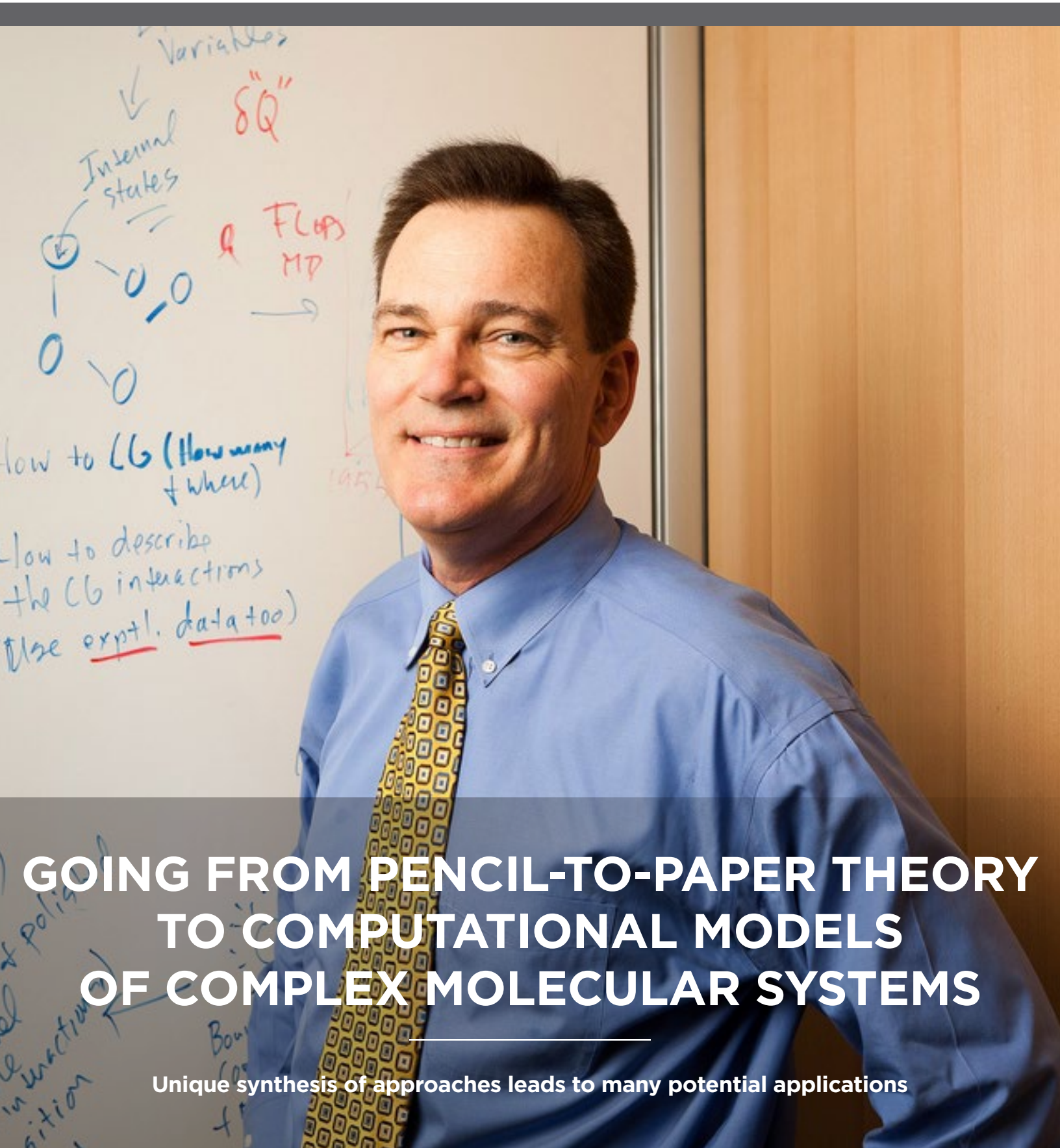
the chemists club

Summer 2022

THE UNIVERSITY OF CHICAGO



GOING FROM PENCIL-TO-PAPER THEORY TO COMPUTATIONAL MODELS OF COMPLEX MOLECULAR SYSTEMS

Unique synthesis of approaches leads to many potential applications

Going from pencil-to-paper theory to computational models of complex molecular systems

By Sheila Evans

There is simply no place as good as UChicago to finish out my career.

Greg Voth grew up in a family of physicians. As a self-described "rebellious teen," Voth happened to read the book given to him by his father entitled *Thirty Years that Shook Physics: The Story of Quantum Theory* which shook his world. "I realized that individual people could positively impact the world," said Voth. While maintaining straight As throughout college, Voth faced the decision of becoming either a doctor or a scientist as he neared graduation. He chose the path of research and dedicated his studies to advanced math and physics. The University of Chicago had an early impact on his research interests, as Voth became fascinated with the work of Dr. Eric Heller, who pursued his postdoctoral studies at UChicago. "Heller knew to bring the computer in at key places in the research," said Voth. During his graduate studies at Caltech, Voth found himself mainly to his own devices and doing research largely on his own. "That freedom essentially led me to be 'self-trained," said Voth. "But, it also led to a certain fearlessness in approaching new problems to solve."

Voth's research took off as he went from classical pencil-to-paper mathematics and theory to incorporating computer calculations. He wanted to demonstrate a new way of solving problems in the field of chemistry, so he tried to address an issue called "the multiscale problem" that still often evades understanding. To find valuable problems to solve, Voth had two criteria, "it has to be something important that no one else has solved," and over time he also wanted to study viruses and other complex biomolecular systems that have enormous implications for human health and disease. The area of research Voth has helped to pioneer is called "Multiscale Theory and Simulation," which uses computational methods to study complex systems along with the underlying mathematical theory. Voth's goal was also to develop a general methodology that would address a large class of problems so that when you solve one, you can apply the approach to others.

After his time as a Professor at the University of Utah, Voth joined the University of Chicago in 2010. "UChicago has a great tradition in theoretical chemistry with pioneers such as Stuart Rice and R. Stephen Berry, so joining the faculty was exciting," explained Voth. Once here, Voth became involved in the James Franck Institute, the Institute for Biophysical Dynamics, and also established the Chicago Center for Theoretical Chemistry. "There is simply no place as good as UChicago to finish out my career," said Voth.

Voth has trained over 200 graduate students at this point in his career. "I learned from my own experiences working in different areas of theoretical chemistry," said Voth, "I tell my students to broaden their training because it will make them better scientists." Graduate students in the Voth group also have the space to solve their problems: "I want them to feel like they aren't just a pair of hands."

"Many things aligned that led me to where I am today," reflected Voth. "I wanted to make a difference in the world, and I was self-taught, pretty darn fearless, and fortunate to have exposure to early thinkers in the field." He hopes that his legacy in the field of chemistry will be in the creation of new ways to attack complex problems using a combination of computational and theoretical methods and, most important of all, the mentorship he has provided to his many graduate students and postdocs.

UChicago Distinguished Chemistry Alumna: Zhenan Bao

By Sheila Evans

Zhenan Bao became acquainted with UChicago from an early age, "My mother was a visiting scholar here, so I already knew about UChicago when I grew up in China. I immigrated to America and settled in Chicago during college." Bao joined Professor Luping Yu's group for her graduate studies. "I was very fortunate. He was the first faculty member in the Department that studied polymer chemistry, which I had interest in because of a prior summer undergraduate research experience," said Bao. Doing materials research in the early 1990s was particularly challenging due to the limited shared characterization facilities available. "Luping encouraged me to reach out. I found an X-ray diffraction tool in the Geophysical Sciences department across the street. Atomic force microscopy just became commercially available, and Luping helped to connect me with a collaborator in the medical school to use the tool," explained Bao, "Those experiences were essential for me to learn about interdisciplinary research. They helped me to practice reaching out and collaborating."

Bao received a job offer from Bell labs at the end of her Ph.D. and later became a Distinguished Member of the Technical Staff. "The collaboration skills I learned at UChicago helped me excel at Bell Labs. What really stood out in my experiences in Bell Labs was the mentorship from colleagues and the highly collaborative environment," said Bao. At Bell Labs, Bao established her independent research on organic electronic materials. She developed material design concepts for flexible displays that could fold and bend, including the world's first flexible electric paper switched by materials she invented.

After moving to Stanford University in 2004, Bao set the goal to create materials and devices that would directly impact human lives, such as helping patients to regain a sense of touch back into a lost arm or hand. "As a materials chemist, I found human skin fascinating because it can sense the environment, and generate electrical signals to communicate with the brain. At the same time, it is naturally flexible, stretchable, and biodegradable in ways that electronics don't have," explained Bao. This fascination turned into a new field of research called "skin-inspired organic electronics" by Bao.

Bao is currently the K.K. Lee Professor of Chemical Engineering and, by courtesy, a Professor of Chemistry and a Professor of Material Science and Engineering at Stanford University. Bao founded the Stanford Wearable Electronics Initiate (eWEAR) in 2016 and serves as the faculty director. She co-founded C3 Nano, Inc., and PyAmes, and serves as an Advising Partner of Fusion Venture Capital. She also mentored numerous students on translating their inventions into start-ups.

To recognize her accomplishments, Prof. Bao and received the UChicago Distinguished Chemistry Alumna Award at an event Wednesday, August 24th, 2022. "I feel extremely honored by this award. UChicago Chemistry is where I learned to be a researcher," said Bao. "To be recognized and confirmed by this place is very special."

A Conversation with Meishan Zhao: Shaping the Undergraduate Lab Experience

By Sheila Evans

The teaching labs are one of the defining features of the Undergraduate Chemistry experience. What does it look like now?
We have expanded significantly over the past years and now have roughly 600 students in the chemistry teaching labs with multiple general chemistry lab sections, serving students in three chemistry sequences: introductory, comprehensive chemistry, and honors chemistry.

What are the benefits of having this "three-layered" approach in general chemistry?
Students come to UChicago with mixed science and math backgrounds. The "three-layered" approach enables us to provide an accessible and appropriately challenging curriculum for all students. The introductory classes are designed to accelerate learning and tailored to support student needs, featuring a slightly different course setting, smaller class sizes, and additional problem-solving sessions. Meanwhile, students who come to UChicago as declared science majors with AP5-level backgrounds in math and chemistry will also have the opportunity to satisfy their curiosity at an appropriate class level. Our goal is to provide a world-class education for all students. By the 3rd academic quarter, introductory class students will have caught up to their peers in their foundational knowledge and will join the comprehensive section. This approach encourages more students to consider further education in sciences and pursue a career in STEM.

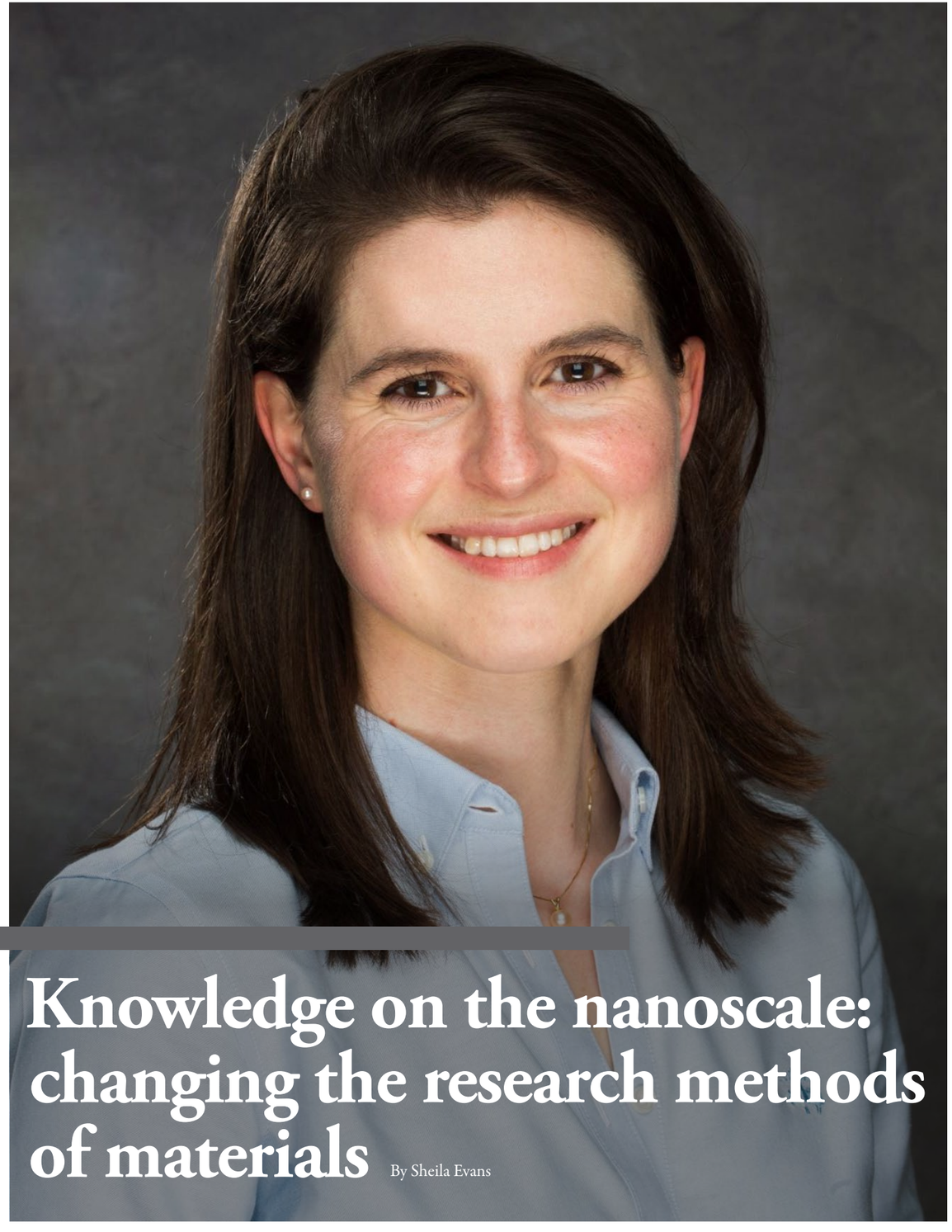
What is the experience like for the teaching assistants?
Teaching assistants (TAs) are essential for students learning and play the most crucial role in undergraduate labs and communication with the students. TAs' performance shapes the outcome of the class, including how well students can learn the material, and as role models who can inform students' perception of chemistry and STEM at large. So, to make a critical transition from student to teacher, all graduate student TAs undergo an intensive training program before taking on students. Many TAs are new to teaching, so we provide all the requisite training to ensure they are prepared for their teaching responsibilities. Besides the required professional training, we also refresh the TAs on the chemistry lab experiences and techniques by leading them through lab experiments, lab safety protocols, and practice discussions. We appreciate our TAs and how vital their contributions are to teaching the undergraduate labs, so we strive to take good care of our TAs. For instance, mental health was an issue nationwide that was especially prominent during the pandemic, and we are mindful of our TAs' work-life balance. We care about the overall well-being of our TAs, their mental health, and their career development.

What is the ultimate goal of lab courses?
Our students are an intelligent young group of people at UChicago, and we owe it to them to provide them with the best learning experience in chemistry regardless of their chosen major. Our hope is that

It is fulfilling and rewarding to work with students in the lab and see them progress daily.

by going through the chemistry classes and the teaching labs, students have a great experience learning chemistry. We hope to inspire them in their STEM curiosity and enhance their desire to take more chemistry classes. Every student has the potential to be a genius if appropriately taught, so we want to give all of them the confidence and chance to reach their potential. As an essential part of the chemistry community in developing the next generation of scientists and engineers, it is fulfilling and rewarding to work with students in the lab and see them progress daily.

Is the Department of Chemistry involved with other programs?
Outside regular classrooms, the department actively provides extensive services to the community, leading or contributing to various outreach activities. Many faculty actively work on outreach and community services, training local high school students in their research labs. Currently, Prof. Sarah King and Prof. John Anderson from the chemistry side are leading the *South Side Science Festival*, a comprehensive campus-wide science fair. The department supports and contributes to the UChicago *Quantum Community Impact Initiative* to serve and inspire participation from the community in quantum education and research for the next generation of scientists. The department also contributes, enthusiastically and dynamically, to the various college community service programs, including the *Collegiate Scholars Program* for middle school and high school students from the CPS Chicagoland community, the *Chicago Academic Achievement Program* for the incoming first-generation, low-income, and other underprivileged students, and the *SESAME* program for the training of Chicagoland CPS science teachers. The graduate and undergraduate student groups also perform outreach activities, such as leading students from the local community on-campus touring and visiting local schools to provide science lectures and demonstrations. We want to promote chemistry education, enhance community awareness, and raise science confidence in our local community. I am proud to have participated in and served in several of these aforementioned programs.



Knowledge on the nanoscale: changing the research methods of materials

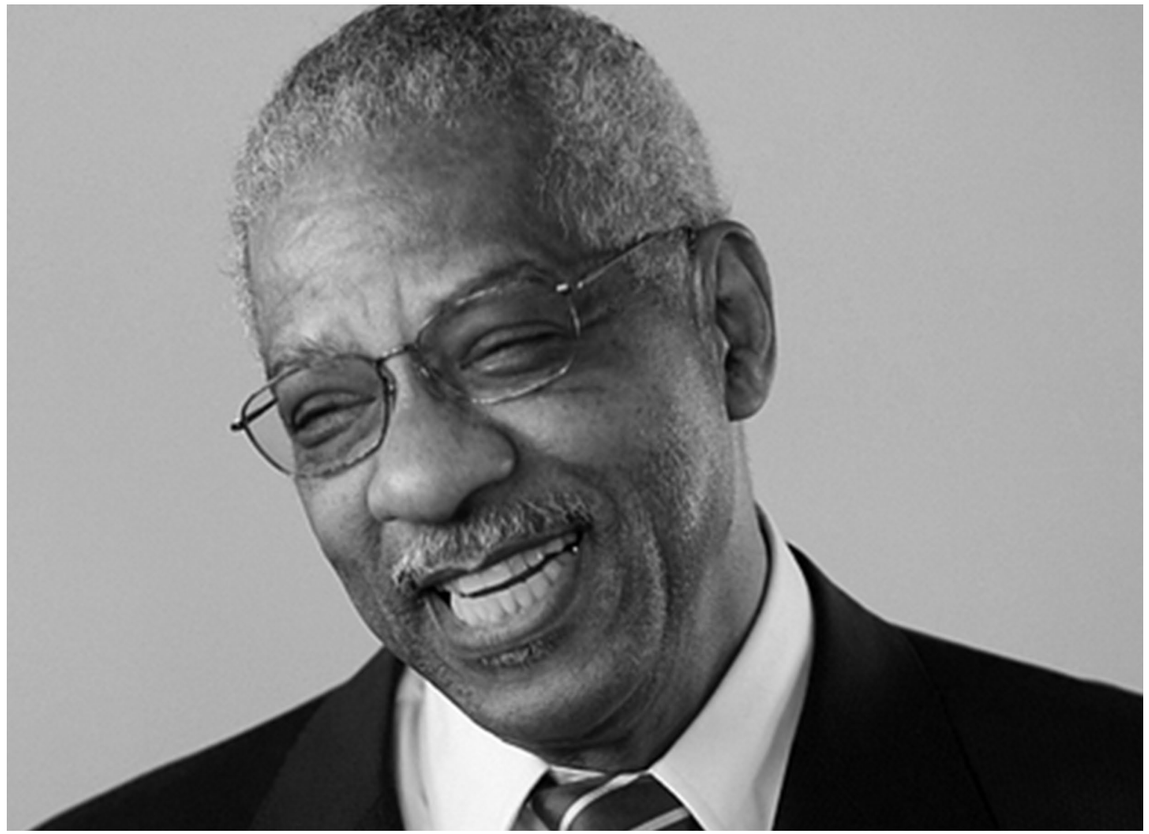
By Sheila Evans

I love collaborative work and the people side of science

Two-dimensional materials hold exceptional promise in upending the scaling problem in electronic devices and offer unique physics and chemistry critical for next-generation energy and information conversion and transport. Sarah King studies 2D materials and their potential applications. Her research focuses on how nanoscale morphology in low-dimensional materials determines their functional properties.

To get down to the nanoscale, King uses a photoemission electron microscope and ultrafast lasers. When probed on the nanoscale, it becomes evident that 2D materials and their electronic structure and dynamics can vary substantially. You can probe the formation of ferroelectric and ferromagnetic domains on the nanoscale under different strain conditions. Ultrafast energy transfer and transport on the nanoscale can depend on the alignment of molecular crystalline domains. There is a causal relationship between nanostructure and functionality, so strategies to tune the nanostructure of materials can unveil new properties.

Probing the electronic structure and properties on the nanoscale is also critical for characterizing new, potentially exciting, materials that we can't make large enough samples of for investigating their properties in more conventional ways. "How do you create a prototype based on a new material if it takes five years to figure out if the material does what you predict it does?" asks King, "We are trying to close that loop." In addition to the experiments going on in King's lab at UChicago, King also performs experiments out at Argonne, where the Ultrafast Electron Microscope facility can be used to investigate the nanoscale dynamics of phonons in materials in real-time. Much of the research previously conducted in materials chemistry using advanced spectroscopy and ultrafast dynamics focused on model systems. "I was very frustrated during previous research when moving beyond model material systems because the disorder made it incredibly challenging to disentangle the dynamics of the materials," explained King. "The connection between model materials and the messy world of chemistry is a big open question in chemistry writ large." New technology and conversations among colleagues open new questions



Thomas W. Cole, contributor to synthesis of cubane, higher education leader, 1941-2022

Dr. Thomas W. Cole, Jr. (PhD '66), an alumnus of the Department of Chemistry who significantly contributed to the first synthesis of cubane, and a leader in higher education died April 14. He was 81 years old.

As a PhD student, Cole worked with his advisor, Professor Emeritus Phillip Eaton, to synthesize cubane. Before this work, cubic carbon-based molecules were considered to be too highly strained to exist, so the synthesis of cubane was expected to be impossible. Cubane and similar hydrocarbons are useful for controlled energy storage because they can store large amounts of energy in small spaces. "Tom initialized the decades-long investigation of the incredible chemistry of cubane," said Eaton.

Cole was the first graduate student to work with Eaton, and they developed a good professional relationship. As Cole reflected in a 2006 interview with the HistoryMakers, "He turned out to be a very good major professor, had my interests at heart, and really wanted to see me continue to do well".

After earning his PhD in Organic Chemistry from UChicago, Thomas W. Cole took leadership positions at multiple universities. Cole was named President of Atlanta University and of Clark University in 1988, then the founding President of the combined Clark Atlanta University. He served as its president until 2002. He came out of retirement to serve as chancellor of the University of Massachusetts Amherst in 2007-2008.

"Tom was a true gentleman, liked and respected by all," said Eaton.

Congratulations

DEGREES AWARDED

PhDs

Spring Quarter 2022

Elizabeth Bain (Engel)
Kate Berger (Levin)
Jan-Niklas Boyn (Mazziotti)
Kyle Cassaidy (Rawal)
Simon Ewing (Mazziotti)
Jake Higgins (Engel)
Maggie Kelty (Anderson)
Lawson Lloyd (Engel)
Jia-Ahn Pan (Talapin)
Aleksander Prominski (Tian)
Tian Qiu (Dickinson)
Huw Rees (Picirrilli)
Ben Slaw (Lee)
Scott Smart (Mazziotti)
Laura Tociu (Vaikuntanathan)
Jiaxin Xie (Dong)
Jiaze Xie (Anderson)

MS in Chemistry

Spring Quarter 2022

Simon Ewing
Shubhashree Pani
Bryan Reynolds
Ahit Kaan Tarhan
Eric You

Summer Quarter 2022

Theint Nandar Aung
Matthew Zajac

BA or BS in Chemistry

Spring Quarter 2022

Emmanuel Amoako BS
Anisul Arefin BS
Ian Baram BS
Marta Beramendi-Conde BS
Josephine Buclez BA
Justin Chen BS
Clementene Clayton BS
Maxwell Cohen BS
Remi Dado BS
Alex Delhumeau BS
Joel Gardner BS
Carl Gibson IV BS
Eduardo Gonzalez Santiago BS
Zachary Green BS
Ellen Guerra BA
Alexandra Hinkle BS
Benjamin Kash BS
Marie Yang-Ji Kim BA
Isabel Korpas BS
Maximilian Korsun BS
Sophia Ho Lam BS
Alexander Liang BS
Bernardo Llaneta BS
Vivian Lu BS
Daniel Mansour BS
Rocco Molinelli BS
Sofia Natividad BS
Michelle Nguyen BS
Kavita Parekh BS
Jennifer Yin Phu BA
Aubrianna Ramsland BS
Benjamin Lee Ratchford BS
Samuel Russo BS
Omar Salinas BS
Jesse Santana BS
Stella Simotas BA
Zihao Sui BS
Ahit Kaan Tarhan BS
Maxwell Taub BS
Jacob Wolf BS
Yuhan Xu BS
Eric You BS
Zachary Yung BS

Summer Quarter 2022

Jordan Klevens BS
Chloe Mesa BA

NOTABLE AWARDS 2022-2023

Chuan He earns Faculty Award for Excellence in Graduate Teaching and Mentoring

U.S. Department of Energy Awards $12.5 million to UChicago for new Energy Frontier Research Center Led by **Laura Gagliardi** and includes **John Anderson** and **Anna Wuttig**

THE DEPARTMENT OF CHEMISTRY

continues its mission of research and education with the help of alumni and friends like you. You can be a catalyst in the process of scientific discovery by making a gift to the department. Donate at chemistry.uchicago.edu/giving-to-chemistry, selecting **Chemistry** under **Area of Support** and listing the fund to which you would like to contribute under **Special Instructions**, or send a check to:

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Attn: Laura Baker
5735 South Ellis Avenue Chicago, IL 60637

The students, faculty, and staff of the department are grateful for your support.

CHEMISTRY EVENTS The most up-to-date information on Department of Chemistry lectures and events can be found online at events.uchicago.edu/chem/index.php.

LET'S KEEP IN TOUCH The Department of Chemistry is updating its records. Send your current e-mail address and other contact information to chemistsclub@uchicago.edu.

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the chemists club

Summer 2022

Dear friends,

We have enjoyed a lovely summer in Chicago this year, with many bright spots and exciting developments for the Department of Chemistry! The biggest event was the ACS National Meeting that took place in August at McCormick Place. UChicago Chemistry was well represented at the meeting, and many of our faculty and students presented their latest research. The meeting also afforded the opportunity to reconnect with the many alums who were in town. During the week, the Department recognized Zhenan Bao (PhD '95), Professor and Chair of Chemical Engineering at Stanford, with a Distinguished Chemistry Alumna Award. Zhenan delivered an inspiring lecture to an audience of over 100 on her pioneering work on human-skin-inspired flexible organic electronic materials and devices.

Members of the Department faculty continue to flourish in both mentorship and research. Chuan He won the well-deserved Faculty Award for Excellence in Graduate Teaching and Mentoring. Laura Gagliardi's work on the EFRC Catalyst Design for Decarbonization Center (CD4DC) received funding from the Department of Energy. Our research community is becoming more robust with burgeoning activity from the new Origins of Life initiative led by Jack Szostak. His new labs in Searle are nearing completion, and we look forward to exciting new insights on the prebiotic chemistry that led to living systems.

Summer is also the time to connect with our surrounding community and neighbors. Sarah King is part of the leadership putting together the first annual South Side Science Festival, a celebration of science for all ages. The event, which is being held on September 17th, will feature live experiments and demonstrations presented by our Department members. The summer also brought sad news of the loss of Dr. Thomas W. Cole, Jr. (PhD '66), a celebrated alumnus and accomplished higher education leader.

We look forward to another fruitful and inspiring academic year on campus and welcome the new energy that our students and postdocs bring to the Department!

Best regards,

Viresh Rawal
Professor and Chair